Chlorthal-dimethyl 1861-32-1 | DTXSID0024000

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Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 1.55e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.76e-01

Confidence level: 5.45e-01

Nearest Neighbors from the Training Set

Image not found

Ampyrone
Measured: 3.58
Predicted: 3.88e-01

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1-Benzoylazepan-2-one Measured: 6.81e-03 Predicted: 1.14e-01 Image not found

4-Dimethylaminoantipyrine **Measured:** 2.35e-01

Predicted: 4.06e-01